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Aquabis[*N*-(5,7-dibromoquinolin-8-yl)-4-methylbenzenesulfonamidato-κ^2N,N']zinc(**II**)

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Key indicators

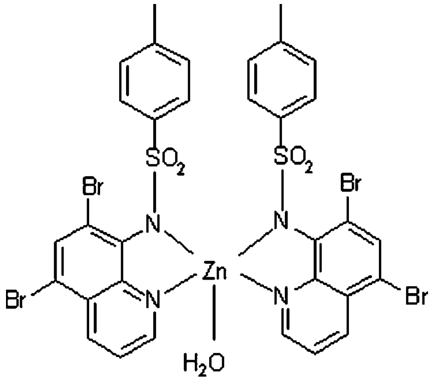
Single-crystal X-ray study
T = 299 K
Mean σ(C–C) = 0.012 Å
Disorder in main residue
R factor = 0.047
wR factor = 0.123
Data-to-parameter ratio = 13.5

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

The molecule of the title compound, $[Zn(C_{16}H_{11}Br_2N_2O_2S)_2(H_2O)]$, occupies a special position on a twofold axis. Zinc is square-pyramidal coordinated by the N atoms of the quinoline and the sulfonamide groups and one water molecule. The water molecule has one weak intermolecular hydrogen bond to a sulfonyl O atom.

Comment

Metal complexes of heterocyclic sulfonamides have been investigated as carbonic anhydrase inhibitors (Supuran & Clare, 1998). On the other hand, 8-aminoquinolinesulfomidate derivatives have been used as powerful tools to detect and measure the available zinc(II) within cells (Fahrni & O'Halloran, 1999). The investigation of the coordinating behavior of these compounds is of interest in connection with their physiological role, as well as their use as chelating reagents for the selective recovery of metal ions (Högberg *et al.*, 1985).



(I)

As part of our study of the 8-aminoquinolinesulfomidate derivatives as fluorescent materials (da Silva *et al.*, 2006*a*,*b*,*c*), the structure of the title compound, (I), was determined. In (I), the Zn atom and the water O atom occupy special positions on a twofold axis. The zinc is five-coordinated by the quinoline N atoms, the sulfonamide N atoms and the water molecule. The Zn1—N2 bond involving quinoline atom N2 is significantly longer than Zn1—N1 bond involving the sulfonamide group. Selected bond distances and angles around the central Zn atom are given in Table 1. Quinolinesulfomidate ligates through the sulfonamide and the quinoline N atoms, forming a five-membered ring with the Zn atom. The water molecule has one weak intermolecular hydrogen bond to a sylfonyl O atom (Table 2).

Experimental

The ligand *N*-(5,7-dibromoquinolin-8-yl)-4-methylbenzenesulfonamide was obtained according to the procedure previously described (da Silva *et al.*, 2005). Compound (I) was prepared by a literature procedure (Macías *et al.*, 2003). Single crystals of (I) suitable for X-ray data collection appeared after a few days from a methanol solution.

Crystal data

$[Zn(C_{16}H_{11}Br_2N_2O_2S)_2(H_2O)]$
M_r = 993.68
Trigonal, $P3_221$
a = 15.8969 (9) Å
c = 12.1289 (9) Å
V = 2654.5 (3) Å^3
Z = 3
D_x = 1.865 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 5.37 mm^{-1}
T = 299 (2) K
Prism, light green
0.28 × 0.10 × 0.10 mm

Data collection

Oxford Diffraction Xcalibur diffractometer with Sapphire CCD detector
φ scans
Absorption correction: analytical (*CrysAlis RED*; Oxford Diffraction, 2004)
T_{min} = 0.272, T_{max} = 0.583
20412 measured reflections
3491 independent reflections
2807 reflections with $I > 2\sigma(I)$
R_{int} = 0.039
θ_{max} = 26.3°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.123
S = 1.13
3491 reflections
259 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0676P)^2 + 0.0141P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.049
$\Delta\rho_{max}$ = 0.55 e Å^{-3}
$\Delta\rho_{min}$ = −0.45 e Å^{-3}
Absolute structure: Flack (1983), 1485 Friedel pairs
Flack parameter: −0.004 (14)

Table 1
Selected geometric parameters (Å, °).

N1—Zn1	2.084 (4)	O3—Zn1	1.984 (7)
N2—Zn1	2.219 (6)		
O3—Zn1—N1	125.02 (12)	N1—Zn1—N2	76.83 (19)
N1^i—Zn1—N1	109.9 (2)	N1—Zn1—N2^i	95.19 (18)
O3—Zn1—N2	96.87 (14)	N2—Zn1—N2^i	166.3 (3)

Symmetry code: (i) $x-y, -y, -z+\frac{1}{3}$.

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O3—H3O···O2^{ii}	0.84 (2)	2.66 (7)	3.126 (7)	117 (5)

Symmetry code: (ii) $y, x, -z$.

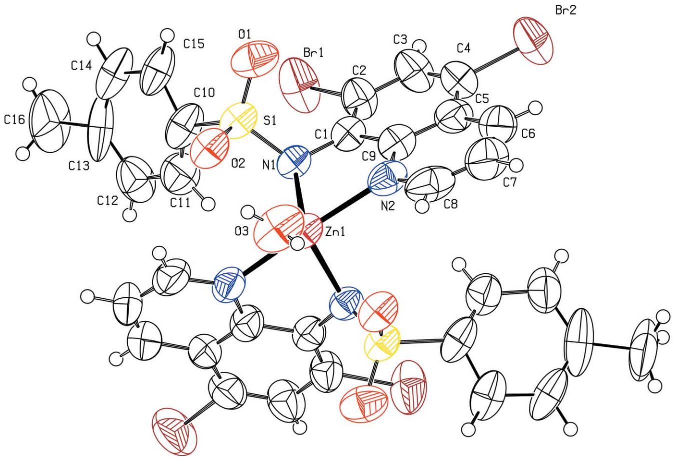


Figure 1
Molecular structure of (I), showing the atom labeling and displacement ellipsoids drawn at the 50% probability level. The minor disorder components are not shown. Atoms without labels are related to corresponding atoms with labels by the symmetry operation ($x-y$, $-y$, $\frac{1}{3}-z$).

The O-bound H atom was located in a difference map and was refined with restrained geometry (Nardelli, 1999), *viz*. the O—H distance was restrained to 0.85 (2) Å and the H···H distance was restrained to 1.365 (2) Å, thus leading to the angle of 107°. The other H atoms were positioned with idealized geometry using a riding model with C—H = 0.93 Å (aromatic) and 0.96 Å (methyl). All H atoms were refined with isotropic displacement parameters (set to 1.2U_{eq} of the parent atom). C13—C15 of the phenyl ring and C16 of the methyl group are disordered and were refined using a split model. The corresponding site-occupation factors were fixed at 0.5.

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2004); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2004); data reduction: *CrysAlis RED*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003) and *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

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